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TOPS: A Multigroup Opacity Code

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By

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ABSTRACT

From T-4 Opacity Library Data, the TOPS code calculates multigroup opacities that can be written in a variety of formats for use in radiation transport codes. Arbitrary mixture of any elements for which OPLIB data exist is supported. Versions of the code exist for both the CRAY-1 and the CRAY X-MP.

I. INTRODUCTION

Multigroup radiation transport packages are being developed in increasing numbers. Thus, the need for multigroup opacities from the best available source has become important for the Laboratory. The TOPS code was developed to provide tabulated multigroup opacities based on the data stored on T-4's Opacity Library (OPLIB).[1] It contains a routine, written by Gary Pfeufer of Group X-6 at Los Alamos, that writes the SESAME files. Jack Peterson's (X-7) memory manager and parser are both used by the code. The group mean calculations are carried out by subroutines adapted from the T-4 group mean codes written by Mary Argo.

The opacities can be provided in formats suitable for direct use in existing radiation transport codes. Commands in the TOPS code allow you to specify the desired file format for the data, the photon energy group boundaries, and an arbitrary density grid. Interpolation on temperature is not supported, so user-defined temperature grids are restricted to subsets of the temperature grids for which the OPLIB data are tabulated. You can arbitrarily mix any available OPLIB materials. There are 51 elements for which OPLIB data have been calculated, so most mixtures of interest can be calculated. You can also scale the data by atomic weight to obtain opacities for any isotopes of existing materials.

The time required to run TOPS depends, of course, on the size of the density, temperature, and photon energy grids and on the number of elements in a mixture. Our experience indicates that a single temperature/density point for one material with the default 33 photon energy groups requires approximately 0.01 s of CPU time. The I/O time varies substantially from case to case but seems to average 25% of the CPU time for cases requiring substantial amounts of computation. Thus, for reasonable temperature and density grids of around 30 points each, you can expect a total time of 10 to 20 s for a pure element. Mixtures require an additional 20 to 30 s per material to generate an OPLIB-type file for the mixture before you can perform the group mean calculation.

TOPS contains a routine provided by Gary Pfeufer to fetch the needed OPLIB files from the Common File System (CFS). Since the OPLIB data files are quite large, it takes appreciable time to retrieve them from CFS. Our experience has been that a 10- to 30-min wait can be expected for one complete material.

In Sec. II we give some cautions on the use of the code. Section III contains a description of commands available. Several examples of the use of TOPS are given in Sec. IV and details of the opacity calculation appear in Sec. V. A summary of the STYX[2] file format appears in the appendix.

II. CAUTIONS ON THE USE OF TOPS

As with any code, it is possible to attempt to use TOPS such that it will produce unreasonable results.

Although the code does have a procedure for interpolation on density, there is no provision for extrapolation. Generally, the OPLIB data go to sufficiently low density to meet all reasonable requests. However, at low temperatures, the upper limit on density can be fairly low. Since the code generates a rectangular density/temperature grid, it invariably has densities that exceed the maximum available at low temperatures. In that case, the code calculates a gray opacity from the data at the highest density available and uses that number for the opacity in every photon energy group. Thus, a plot of opacity versus photon energy at a high density and low temperature will be a straight line. A record of densities for which this occurs is written as a text file to TAPE6.

The TOPS code does calculate a gray opacity, but only over the frequency range of the photon groups for which the multigroup opacities were requested. Thus, if you request multigroup opacities for only a small range of photon energies, the gray opacity will not be correct. A reasonable lower bound for photon energies is 1% of the lowest material temperature requested. A good upper bound for photon energies is 30 times the highest material temperature.

A plasma cutoff frequency is calculated in TOPS. Photons below this cutoff are completely absorbed. For any photon energy group with a lower bound lower than the plasma cutoff, the code sets the opacity to the value 1.E10.

As described in the OPLIB data section, Sec. IV, the OPLIB data end at a photon energy equal to 30 times the material temperature. For photon energy groups higher than this limit, the opacity is calculated through extrapolations of bound-free cross sections. At some density/temperature points there can be a slight discrepancy, about 10%, at the matching point.

For some temperature/density points for some materials, a difference in interpolation procedures will cause a small difference between the gray opacity from TOPS and the SESAME opacity. A spline fit to the gray opacities is used to obtain a rectangular temperature/density grid for SESAME. In TOPS, a linear interpolation on the OPLIB data is performed first, then the opacity is calculated from the interpolated data.

III. TOPS COMMANDS

Two versions of the executable code exist, one for the CRAY-1 and one for the CRAY X-MP. They are stored on CFS under the root node /T4OPLIB, with subdirectories CRAY1S and CRAYXMP. A special password is required to access the root node /T4OPLIB. The code is named TOPS under either directory.

All materials are on the root node /T4OPLIB. The file AVMAT under this directory has a summary of materials available to TOPS. For each material there is a name followed by a range of two-digit suffix numbers. The name is keyed to the SESAME material ID corresponding to the 502 table. A directory file is stored with this name. The two-digit suffix numbers are needed because more than one data file is needed per material. For example, hydrogen has the root symbol t15250 and the suffix numbers are 01-04. Thus, the files t15250, t1525001, t1525002, t1525003, and t1525004 are all needed to run TOPS on hydrogen. TOPS contains a routine provided by Gary Pfeufer to fetch files from CFS so that if the data files are not in the local space they will be retrieved, if possible, from CFS. It does take some time to get the files over from CFS. The data files are large, around 1.5 million words decimal each, and they tend to quickly migrate to archival storage.

TOPS does not interpolate on temperatures. You can pick a subset of the temperatures available for a given material. Thus, before defining a temperature grid, you must specify a material so TOPS will have the correct default temperature grid. Any command line may be continued by making the last character on the line an &.

TOPS cannot read commands from an input file. However, several utilities will read commands from a file and pass them to a code. We have been using the XEQ[3] utility. The usage form is simply

XEQ filename

where filename consists of commands for XEQ. In general, the lines in filename start with either a $ or a C in column one. The $ signifies a code to be executed and the C a command to be sent to the code. Thus, the first line in filename would be $TOPS. After this would be commands, each with a C, in column one.

The descriptions of the commands are grouped by command function in the following sections. Section A describes the F and M commands. Commands to set the temperature grid are explained in Sec. B. Section C gives the density grid commands. The photon energy grid commands are given in Sec. D. Section E contains commands relating to the multigroup opacity files. SESAME file commands are described in Sec. F. Commands involving material properties are in Sec. G and all other commands are in Sec. H. Table I lists all commands.

TABLE I

F r_1 sym_1 r_2 sym_2 · · · · · ·
M m_1 sym_1 m_2 sym_2 · · · · · ·
T t_1 t_2 t_3 · · · · · · · · · ·
TINT t_{low} t_{up}
TBY n
R r_1 r_2 r_3 · · · · · · · · · ·
RLOG n r_{low} r_{up}
RLIN n r_{low} r_{up}
G e_1 e_2 e_3 · · · · · · · · · ·
GLOG n e_{low} e_{up}
GLIN n e_{low} e_{up}
MG op
MGF fname
MGID n
SEST T/F
SESF fname
MATID n
IDS T/F
SCALE rscale
ATWT
Z
DAW atwt
MASS T/F
AVMAT
HELP
GO
END

A. The F and M Commands

F r_1 sym_1 r_2 sym_2 · · ·

This command defines the material, a procedure necessary before you use any of the temperature commands. The values of sym must correspond to OPLIB materials that are on the root node /T4OPLIB or that are in your local file space. The file /T4OPLIB/AVMAT has a list of available materials and TOPS has the ability to fetch the needed files from mass. The file AVMAT can be listed by TOPS with the command AVMAT. If the file is not local, TOPS will fetch it from mass. The values of r correspond to number amounts of materials to be mixed. They need not be normalized. TOPS will generate number fractions normalized to 1. For example, you might wish to mix two parts of material t15250 and one part of material t15010. You can accomplish this with the command

F 2. t15250 1. t15010

after which TOPS will ask for a name for the mixture. The name must contain no more than six characters and must begin with an alphabetic character. Suppose it is given the name WATER. TOPS will then perform the mix and store the OPLIB-type data with the file name WATER and display the temperature grid for which data are available. If you had requested only one material, that is, no mixture, there would not have been a request for a file name and the temperature grid would have been displayed immediately. Once you have created the files with name WATER, they are treated exactly as any other OPLIB-type files. You can save them for future use.

A complication arises if you wish to mix a premixed material with another material. For example, suppose you want to mix one part of material t17830 with the material WATER from the example above to form a mixture of one part t17830, two parts t15250, and one part t15010. Of course, you could use the command

F 1. t17830 2. t15250 1. t15010

to obtain the mixture. However, you might wish to use the premixed material WATER. The problem is that the WATER directory file contains number fractions normalized to 1. In other words, it does not contain the number fractions as 2 parts t15250 and 1 part t15010, but rather it has 0.6666667 part t15250 and 0.3333333 part t15010. Thus, to get back to the desired number fractions you must, in effect, un-normalize the number fractions by multiplying by 3. Thus the command

F 1. t17830 3. WATER

will produce the desired mixture. Again, the name for the new material must not contain more than six characters. Thus you could name this new material CWATER but not SEAWATER.

M m_1 sym_1 m_2 sym_2 · · ·

This command is similar to the F command except that the amounts of materials are specified in terms of mass fractions. The complication in mixing premixed materials with the F command does not arise with the M command since masses are being mixed. Thus, if you wanted to mix 1 g of material T17830 with 1 g of the premixed material WATER from the example above, the command

M 1 t17830 1 WATER

would produce the desired mixture.

B. Temperature Grid Commands

T t_1 t_2 t_3 · · ·

The T command allows specific temperatures (in keV) to be entered. TOPS compares these temperatures to the default grid for the material and keeps only temperatures that match ones in the grid. The valid temperatures are then displayed. The T command will not function until a material is defined. When you define a new material, the temperature grid is reset to the default temperature grid of the new material.

TINT t_{low} t_{up}

This command lets you keep all grid temperatures in the interval between t_{low} and t_{up}. The resulting set of temperatures is displayed. The TINT command will not function until you define a material. When you define a new material, the temperature grid will be reset to the default temperature grid of the new material.

TBY n

This allows you to thin the default temperature grid. For example n = 2 will pick every other temperature. The resulting set of temperatures is displayed. The TBY command will not function until you define a material. When you define a new material, the temperature grid will be reset to the default temperature grid of the new material.

C. Density Grid Commands

R r_1 r_2 r_3 · · ·

The R command lets you specify densities in g/cm^3. TOPS will interpolate on densities but will not extrapolate. If a density is greater than OPLIB has available at a given temperature, TOPS will use the highest density point available from the OPLIB data. These data will then be collapsed to a gray opacity and that value will be used as the group mean opacity for every group for the requested density. A record of the densities for which this occurs is written to TAPE6. The maximum number of densities allowed is 100. The default density grid consists of 17 densities with logarithmic spacing between 0.005 and 500 g/cm^3.

RLOG n r_{low} r_{up}

The RLOG command lets you set up a logarithmic grid of n densities between r_{low} and r_{up}. The procedure described in R above is used on densities higher than available OPLIB densities.

RLIN n r_{low} r_{up}

The RLIN command is similar to the RLOG command except that a linear grid is used.

D. Photon Energy Grid Commands

G e_1 e_2 e_3 · · ·

The G command lets you enter photon energy group bounds in keV. Note that there must be two bounds to define one photon group. Currently there is an upper limit of 1000 photon energies. TOPS contains a default photon energy grid with 33 groups between 0.00001 and 300 keV. It should be mentioned that TOPS calculates a plasma cutoff photon energy. If the lower group bound for a group lies below the cutoff, the opacity for that group is set to 1.e10.

GLOG n e_{low} e_{up}

The GLOG command lets you set up a logarithmic grid of photon energies.

GLIN n e_{low} e_{up}

The GLIN command lets you set up a linear grid of photon energies.

E. Multigroup Opacity File Commands

MG op

The MG command lets you specify what to do with the multigroup opacities. The option S writes a STYX[2] file. The appendix describes this file. Gary Pfeufer has written an interface for accessing and manipulating data from a STYX file.[4] The option M writes a sequential binary file to TAPE11. The option T writes a BCD file to TAPE7, which is formatted for use in the CURVES[5] code. BOTH combines the S and M options, ALL

combines the S, M, and T options, and F turns off all the multigroup file options. The default is to write a STYX file to a file named STYXU. Files TAPE7 and TAPE11 can be renamed on the execute line by

TOPS Tape7=fname1 Tape11=fname2 / t p

MGF fname

This command lets you specify the file name to which the STYX file will be written. The default name is STYXU.

MGID n

This command lets you specify an identification number for the multigroup opacities for the current material. It must be an integer between 10000 and 19999. The default value is 19000. If IDS is not set to false, MATID will automatically be set equal to MGID.

F. SESAME File Commands

SEST T/F

This command lets you specify whether to write a SESAME type 502 table. The option is either T for true or F for false. The default is T.

SESF fname

This command lets you specify the name of the file to which the SESAME-type data are to be written. The default file name is SESAMEU.

MATID n

This lets you specify an identification number for the current material for the SESAME-type file. The number must be between 10000 and 19999 since only a 502 table is being written. The default is 19000. If IDS is not set to false, MGID will automatically be set equal to MATID.

IDS T/F

If IDS is set to true, when you enter a new MATID, MGID will be set to the same value and vice versa. If IDS is set to false, MGID and MATID are totally independent. The default is for IDS to be true.

G. Material Property Commands

SCALE rscale

The scale command lets you scale opacities for different isotopes. The factor rscale is defined as the ratio of the desired atomic weight to the actual atomic weight of the available material. For example, to obtain opacities for tritium from hydrogen, you would use the factor rscale=3. It is possible to find the atomic weight of the current material with the ATWT command.

ATWT

This command has no arguments. It simply displays the atomic weight of the current material.

Z

This command has no arguments. It simply displays the z of the current material.

DAW atwt

This command lets you set the scale factor without having to form the ratio explicitly. The number atwt is the desired atomic weight. For example, if you wanted the opacities for carbon 13 you would use the data files for carbon and the DAW command with the atwt set to 13.

H. Miscellaneous Commands

MASS T/F

The mass command turns the mass fetch command on or off. The default is to attempt to fetch files from mass.

AVMAT

The AVMAT command displays the currently available materials.

HELP

The HELP command, with no argument, simply lists the available commands with no explanation. You can obtain information about a particular command by typing HELP command, where command is the name of the command for which you want information.

GO

This command initiates the group mean routines in TOPS.

END

If this command is not self-explanatory, please do not attempt to run TOPS.

IV. EXAMPLES

A. Single Element, Default Values for Parameters

The simplest case is that of a single element using the default temperature, density, and photon energy grids. We illustrate with material T15250 (Fig. 1.).

For this case all the data files were local, so TOPS did not need to retrieve any files from CFS. Only three commands were used: F, GO, and END. On completion, the files SESAMEU and STYXU would be in your local file space.

B. Simple Mixture, Default Values for All Parameters

This case illustrates mixing two OPLIB materials (Fig. 2.).

Note that you can use any name for the mixture data as long as the name is six or fewer characters and the first character is alphabetic. Also note that TOPS will not allow use of the same material number more than once on either SESAMEU or STYXU. Since both of those files are random access with a directory section at the beginning, it is easy to check the existence of material numbers. This is not true for the file written to unit 11, which is a sequential file. Thus, no checks are performed on material numbers on that file and you must be careful to change the MGID each time you add a material.

C. Setting Temperature, Density, and Photon Energy Grids

We now illustrate using various commands to set up a variety of temperature, density, and photon energy grids (Fig. 3.).

Note that if a temperature-based command gives an empty set of temperatures, the code reverts to the default grid. If you request too many densities or photon energies, the number is reset to the maximum allowed. Redefining a material resets the temperature grid but does not change the density or photon energy grid.

V. DETAILS OF THE OPACITY CALCULATIONS

Section A describes the OPLIB[1] data. Section B gives details of the group mean calculation. The method used to extrapolate beyond u = 30 is described in Sec. C and mixtures are discussed in Sec. D.

```
tops
This version of TOPS was last modified on 6/20/85.
It contains an expanded help package.
It is version tops-007

command
? f 1 t15250
f 1 t15250
temperature grid for t15250
 1.000e-03 1.250e-03 1.500e-03 2.000e-03 2.500e-03 3.000e-03 4.000e-03
 5.000e-03 6.000e-03 8.000e-03 1.000e-02 1.250e-02 1.500e-02 2.000e-02
 2.500e-02 3.000e-02 4.000e-02 5.000e-02 6.000e-02 8.000e-02 1.000e-01
 1.250e-01 1.500e-01 2.000e-01 2.500e-01 3.000e-01 4.000e-01 5.000e-01
 6.000e-01 8.000e-01 1.000e+00 1.250e+00 1.500e+00 2.000e+00 2.500e+00
 3.000e+00 4.000e+00 5.000e+00 6.000e+00 8.000e+00 1.000e+01 1.500e+01
 2.500e+01 4.000e+01 6.000e+01 1.000e+02

command
? go
go

command
? end
end
```

Fig. 1. Single element using the default temperature, density, and photon energy grids (material T15250).

```
tops
This version of TOPS was last modified on 6/20/85.
It contains an expanded help package.
It is version tops-007

command
? f 1 t13710 1 t15250
f 1 t13710 1 t15250
name for mixture data
? junk
temperature grid for junk
 1.000e-03 1.250e-03 1.500e-03 2.000e-03 2.500e-03 3.000e-03 4.000e-03
 5.000e-03 6.000e-03 8.000e-03 1.000e-02 1.250e-02 1.500e-02 2.000e-02
 2.500e-02 3.000e-02 4.000e-02 5.000e-02 6.000e-02 8.000e-02 1.000e-01
 1.250e-01 1.500e-01 2.000e-01 2.500e-01 3.000e-01 4.000e-01 5.000e-01
 6.000e-01 8.000e-01 1.000e+00 1.250e+00 1.500e+00 2.000e+00 2.500e+00
 3.000e+00 4.000e+00 5.000e+00 6.000e+00 8.000e+00 1.000e+01 1.500e+01
 2.500e+01 4.000e+01 6.000e+01 1.000e+02

command
? go
go

matid 19000. exists on file sesameu
pick a new sesfile or matid or set sest to false
the following matids exist on sesameu
 19000.

command
? matid 19001
matid 19001

command
? go
go

command
? end
end
```

Fig. 2. Mixing two OPLIB materials.

A. Opacity Library Data Description

The T-4 opacity library[1] is the basis for all group mean opacities computed by TOPS. The library contains opacity information for various elements and mixtures. All the SESAME gray opacities have been derived from the T-4 opacity library. For each material opacity, data are tabulated on a piecewise rectangular temperature (T)-degeneracy parameter (η) grid. The degeneracy parameter η is related to the chemical potential and increases with increasing density for a fixed temperature.

The library is based on degeneracy parameter, so the opacity of a mixture may be easily calculated. The temperature grid is presented in Table II and the degeneracy parameter grid is presented in Table III.

TABLE II. Temperature Grid (keV)

.00100	.0100	.100	1.00	10.0
.00125	.0125	.125	1.25	15.0
.00150	.0150	.150	1.50	25.0
.00200	.0200	.200	2.00	40.0
.00250	.0250	.250	2.50	60.0
.00300	.0300	.300	3.00	100.0
.00400	.0400	.400	4.00	
.00500	.0500	.500	5.00	
.00600	.0600	.600	6.00	
.00800	.0800	.800	8.00	

```
tops
This version of TOPS was last modified on 6/20/85.
It contains an expanded help package.
It is version tops-007

command
? tint .05 10.
tint .05 10.
specify a material with the f command

command
? f 1 t15250
f 1 t15250
temperature grid for t15250
 1.000e-03 1.250e-03 1.500e-03 2.000e-03 2.500e-03 3.000e-03 4.000e-03
 5.000e-03 6.000e-03 8.000e-03 1.000e-02 1.250e-02 1.500e-02 2.000e-02
 2.500e-02 3.000e-02 4.000e-02 5.000e-02 6.000e-02 8.000e-02 1.000e-01
 1.250e-01 1.500e-01 2.000e-01 2.500e-01 3.000e-01 4.000e-01 5.000e-01
 6.000e-01 8.000e-01 1.000e+00 1.250e+00 1.500e+00 2.000e+00 2.500e+00
 3.000e+00 4.000e+00 5.000e+00 6.000e+00 8.000e+00 1.000e+01 1.500e+01
 2.500e+01 4.000e+01 6.000e+01 1.000e+02

command
? t .7 .75
t .7 .75
default temperature grid used
 1.000e-03 1.250e-03 1.500e-03 2.000e-03 2.500e-03 3.000e-03 4.000e-03
 5.000e-03 6.000e-03 8.000e-03 1.000e-02 1.250e-02 1.500e-02 2.000e-02
 2.500e-02 3.000e-02 4.000e-02 5.000e-02 6.000e-02 8.000e-02 1.000e-01
 1.250e-01 1.500e-01 2.000e-01 2.500e-01 3.000e-01 4.000e-01 5.000e-01
 6.000e-01 8.000e-01 1.000e+00 1.250e+00 1.500e+00 2.000e+00 2.500e+00
 3.000e+00 4.000e+00 5.000e+00 6.000e+00 8.000e+00 1.000e+01 1.500e+01
 2.500e+01 4.000e+01 6.000e+01 1.000e+02

command
? tby 3
tby 3
   16  temperatures kept
 1.000e-03 2.000e-03 4.000e-03 8.000e-03 1.500e-02 3.000e-02 6.000e-02
 1.250e-01 2.500e-01 5.000e-01 1.000e+00 2.000e+00 4.000e+00 8.000e+00
 2.500e+01 1.000e+02

command
? glog 255 .0001 2.e6
glog 255 .0001 2.e6

command
? rlog 155 .001 5500
rlog 155 .001 5500
too many densities requested - reset to  101

command
? f 1 t15250
f 1 t15250
temperature grid for t15250
 1.000e-03 1.250e-03 1.500e-03 2.000e-03 2.500e-03 3.000e-03 4.000e-03
 5.000e-03 6.000e-03 8.000e-03 1.000e-02 1.250e-02 1.500e-02 2.000e-02
 2.500e-02 3.000e-02 4.000e-02 5.000e-02 6.000e-02 8.000e-02 1.000e-01
 1.250e-01 1.500e-01 2.000e-01 2.500e-01 3.000e-01 4.000e-01 5.000e-01
 6.000e-01 8.000e-01 1.000e+00 1.250e+00 1.500e+00 2.000e+00 2.500e+00
 3.000e+00 4.000e+00 5.000e+00 6.000e+00 8.000e+00 1.000e+01 1.500e+01
 2.500e+01 4.000e+01 6.000e+01 1.000e+02

command
? end
end
```

Fig. 3. Various commands to set up a variety of temperatures, density, and photon energy grids.

TABLE III. Degeneracy Parameter Grid				
−28	−18	−8	5	500
−27	−17	−7	8	
−26	−16	−6	12	
−25	−15	−5	20	
−24	−14	−4	30	
−23	−13	−3	50	
−22	−12	−2	80	
−21	−11	−1	120	
−20	−10	1	200	
−19	−9	3	300	

No data for temperatures less than 0.05 keV are present for high-Z elements (Z>30) and mixtures containing high-Z elements. Also, for such materials the η grid starts at about -25.

In general, data for high values of η are missing for low values of T. As the temperature increases the set of degeneracy parameters becomes more complete.

The data stored at each η,T point consist of reduced extinction (D_t) and scattering coefficients (D_s) tabulated on a fixed grid of 3000 reduced photon energies, u, plus other related quantities.

The reduced photon energy is given by

$$u = \frac{h\nu}{kT} , \tag{1}$$

where $h\nu$ is the photon energy and kT is the temperature. Both must be given in consistent energy units. The 3000 u values range from 0.01 to 30 with a linear spacing Δu of 0.01. Note that the actual photon energies stored for each temperature will be different.

B. Group Mean Calculations

Input to the code the values of temperature, mass density, and the bounds of photon energy intervals for which opacities are desired. Temperatures are restricted to those present on the opacity library (Table II). The code obtains the extinction and scattering coefficients at arbitrary values of mass density by linearly interpolating the opacity library values stored at the bracketing mass densities. The group mean opacities are then obtained by performing a weighted average of the interpolated D coefficients over the specified photon energy bounds.

The Rosseland total group mean opacity is computed from the D's by

$$\kappa_{Rt}^{-1} = \frac{A\rho}{I_R} \int_{u_1}^{u_2} (W_R/D_t)\, du , \tag{2}$$

and the Rosseland absorption group mean opacity is computed using

$$\kappa_{Ra}^{-1} = \frac{A\rho}{I_R} \int_{u_1}^{u_2} (W_R/D_a)\, du , \tag{3}$$

where

$$A\rho = 1.544 \times 10^{-5} (kT) M , \tag{4}$$

W_R is the Rosseland weighting function,

$$W_R = \frac{15}{4\pi^4} u^7 e^{-u} (1 - e^{-u})^{-3} , \tag{5}$$

I_R is the normalization integral

$$I_R = \frac{15}{4\pi^4} \int_{u_1}^{u_2} \frac{u^4 e^{-u}\, du}{(1 - e^{-u})^2} , \tag{6}$$

u_1 is the u value associated with the lower photon energy bound, u_2 is the u value associated with the upper photon energy bound, kT is the temperature expressed in keV, and M is the atomic weight. The reduced absorption coefficients are calculated using

$$D_a(u) = D_t(u) - D_s(u) . \tag{7}$$

The Planck group mean opacity is computed from the D's using

$$\kappa_p = \frac{1}{A\rho\, I_p} \int_{u_1}^{u_2} W_p D_a\, du , \tag{8}$$

where

$$W_p(u) = \frac{15}{\pi^4} e^{-u} \tag{9}$$

and

$$I_p = \frac{15}{\pi^4} \int_{u_1}^{u_2} \frac{u^3 e^{-u}\, du}{1 - e^{-u}} . \tag{10}$$

C. Extrapolation Beyond u = 30

If the photon energy bounds exceed the opacity library limit of u = 30 for a given temperature, the code uses extrapolation to evaluate the D's. Sometimes this

procedure may not join smoothly with the opacity library data because of slight inconsistencies. For u>30 the total cross section is computed from

$$\sigma_t = \sigma_{bf} + \sigma_{ff} + \sigma_s \ , \tag{11}$$

where σ_t is the total cross section, σ_{bf} is the bound-free cross section, σ_{ff} is the free-free cross section, and σ_s is the scattering cross section. All cross sections are in units of cm^2.

To compute the bound-free cross sections, the code scales the neutral bound-free cross sections according to the shell occupation numbers of the ion. Hence the bound-free cross section is given by

$$\sigma_{bf}\ (h\nu) = \sum_j \frac{M_j}{N_j}\ \sigma_j\ (h\nu) \ , \tag{12}$$

where M_j is the occupation number of shell j for the ion, N_j is the occupation number of shell j for the neutral, and σ_j is the cross section for photonization from shell j of the neutral atom. TOPS obtains the ion occupation numbers by filling the most tightly bound shells of the neutral atom according to the number of bound electrons of the ion. The bound-free cross-section fits and neutral occupation numbers are obtained from the TOPSDB file and the number of bound electrons are obtained from the opacity library.

The code computes the free-free contribution to the total cross section by extending the free-free reduced D at $u = 30$ [$D_{ff}(30)$] to higher u values according to the formula

$$\sigma_{ff}\ (u) = \frac{M}{\rho A N_o}\ \frac{D_{ff}(30)}{u^3} \ , \tag{13}$$

where N_o is Avogadros number. $D_{ff}(30)$ is obtained from the opacity library.

To obtain the scattering cross section, TOPS extrapolates scattering cross section at $u = 2900$ and $u = 3000$ to higher values of u. If the extrapolated value exceeds the limit

$$\sigma_s' = \frac{.4Z}{N_o}\ (1 - .21169 \times 10^{-1}\, kT) \ , \tag{14}$$

σ_s is set to the limit σ_s'. In Eq. (14) Z is the average atomic number.

Note that reduced D coefficients may be calculated from cross sections using the formula

$$D(u) = \frac{\rho A N_o}{M}\ \frac{u^3}{(1 - e^{-u})}\ \sigma(u) \ . \tag{15}$$

D. Mixtures

If you specify a mixture of OPLIB materials (an F or M command involving more than one name), OPLIB files are created for the mixture and can be used to calculate group opacities for the mixture. The mixture file will contain only those η and T points common to all constituents. TOPS calculates the reduced D-coefficients for a given η and T by using

$$D(u) = \sum_i r_i\, D_i\,(u) \ , \tag{16}$$

where r_i is the normalized number fraction for material i, D_i is the D-coefficient for material i, D is the D-coefficient for the mixture, and the sum is over all materials. Other parameters stored on the OPLIB files are also adjusted to reflect the composition of the mixture.

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REFERENCES

1. W. F. Huebner, A. L. Merts, N. H. Magee, Jr., and M. F. Argo, "Astrophysical Opacity Library," Los Alamos Scientific Laboratory report LA-6760-M (August 1977).

2. W. Spangenberg, "Structure of Collapsed STYX Data Files," Los Alamos National Laboratory memorandum X-7-84-U200 (July 23, 1984).

3. R. Frank, "XEQ," LASL Utility Routine LTSS-542 (June 1979).

4. Gary W. Pfeufer, "Code Developer's Guide to the STYX Liaison Library: a Software Interface for Accessing and Manipulating STYX Opacity Data," Los Alamos National Laboratory report LA-10381-MS (April 1985).

5. Joseph Abdallah, Jr., "User's Manual for Curves," Los Alamos National Laboratory report LA-8844-M (October 1981).

APPENDIX A
STRUCTURE OF THE STYX FILES (SEE REF. 2)

I. The first 16 words of the directory (The FIDI)

Word	Type	Description
1	I	Length of the FIDI = 16
2	I	Length of the directory section excluding directory filler
3	H	A file type designator = "STYX.COL"
4	H	Signature for the FIDI = "FIIPF\A"
5	I	Number of materials on the file
6	H	Name of the next level of directory = "MIDI"
7	I	The length of the file
8	I	Length of the directory section including directory filler
9	H	Creation date of the data file
10	H	Date of most recent modification
11	I	Version number of the data file
12	H	Version of the code used to create the file
13	H	Name of the data file
14	H	"NOT DEF"
15	H	"NOT DEF"
16	H	"NOT DEF"

II. The first set of 16 words for a specified material (The MIDI)

Word	Type	Description
1	I	Length of MIDI = 16
2	I	Stride from start of one MIDI to the next = 32
3	H	Material identifier
4	H	Signature for the MIDI = "MIIPF\A"
5	I	Number of types of data = 1
6	H	Name of next level of directory = "DSDIR"
7	H	Creation date of this material
8	H	Date of most recent modification
9	I	Version number of the data
10	H	"NOT DEF"
11	H	"NOT DEF"
12	H	"NOT DEF"
13	H	"NOT DEF"
14	H	"NOT DEF"
15	H	"NOT DEF"
16	H	"NOT DEF"

III. The second set of 16 words for a specified material (The DSDIR)

Word	Type	Description
1	I	Length of the DSDIR = 16
2	I	Length of the DSDIR = 16
3	H	"DS530"
4	H	Signature for the DSDIR = "DIIPF\A"
5	I	0
6	H	"NOT DEF"
7	I	6
8	I	Absolute first word address of the data for this material
9	I	Length of the data section addressed by word 8
10	H	"STANDARD"
11	H	"STYXU"
12	H	Creation date of the material
13	H	Date of most recent modification
14	I	Version number of the data
15	H	Version of the code that produced the data
16	H	User number of the person who created the data

The 32 words of sections II and III are repeated for each material.

IV. The first 31 words of the Data Section

Word	Type	Description
1	I	6
2	I	31
3	H	"DS530"
4	H	"STANDARD"
5	I	5
6	I	5
7	H	"TLN530"
8	I	Number of temperatures, NT
9	I	1
10	I	1
11	H	"LN"
12	H	"RHOLN530"
13	I	Number of densities, NR
14	I	1
15	I	1
16	H	"LN"
17	H	"HNULN530"
18	I	Number of group boundaries, NB
19	I	1
20	I	1
21	H	"LN"
22	H	"RASLN530"
23	I	Number of multigroup opacities = NT × NR × (NB-1)
24	I	1
25	I	2
26	H	"LN"
27	H	"RGTLN502"
28	I	Number of gray opacities = NT × NR
29	I	1
30	I	1
31	H	"LN"

After these 31 words are strings of data as follows:

1. A set of natural logarithms of temperatures, NT in number
2. A set of natural logarithms of densities, NR in number
3. A set of natural logarithms of photon energies, NB in number.
4. A set of packed natural logarithms of absorption and scattering multigroup opacities, with temperature being the outer loop, density the next inner loop, and photon group, the innermost loop.
5. A set of natural logarithms of total gray opacities, with temperature being the outer loop and density the inner loop.

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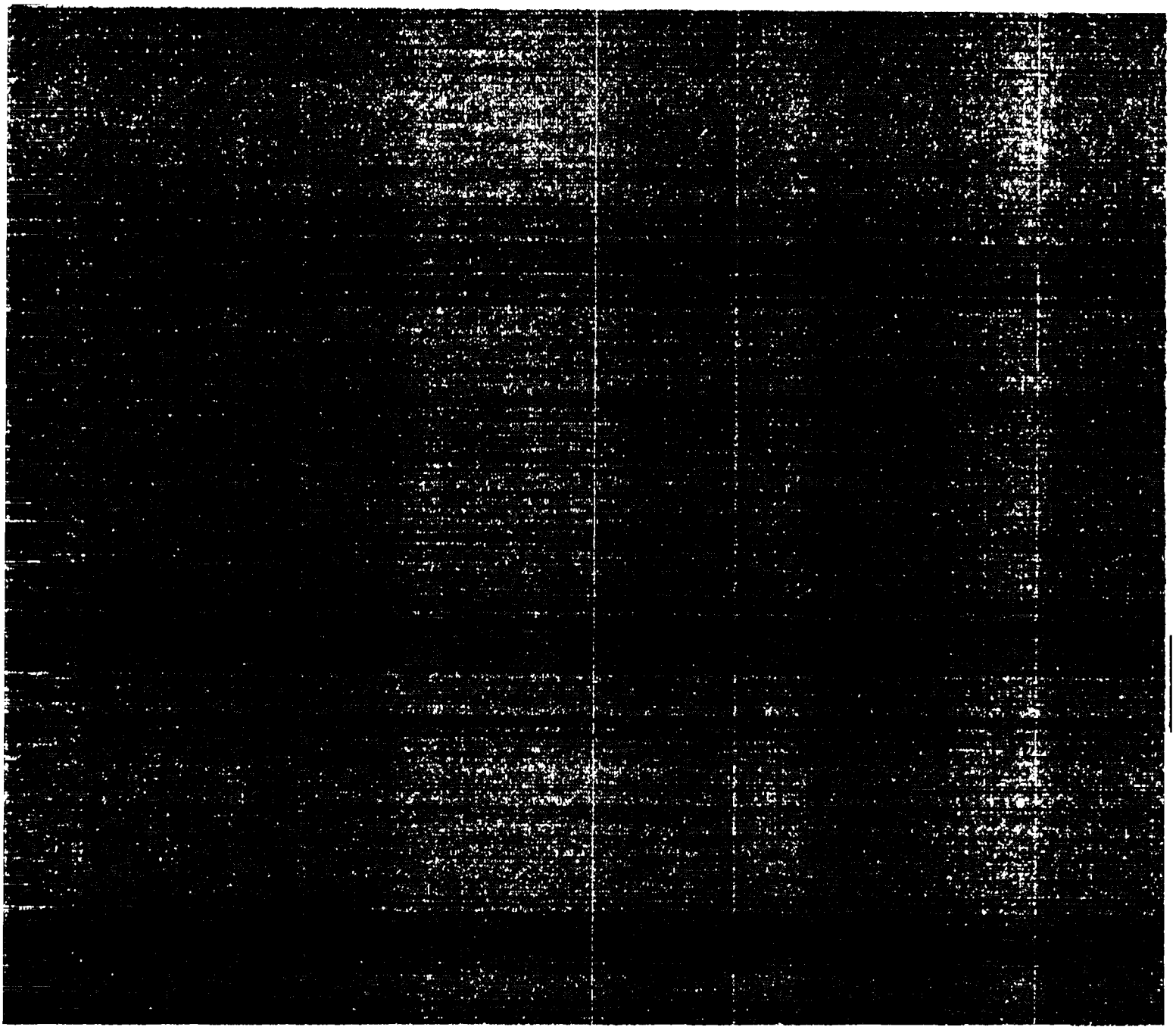

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